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**EXAMINER**: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to Applicant.

**EXAMINER** 

Page 3 of 37 APPLICATION NO. ATTY. DOCKET NO. 1503.1070003 09/934,084 FORM PTO-1449 APPLICANTS Lobanov et al. SUPPLEMENTAL INFORMATION GROUP DISCLOSURE STATEMENT FILING DATE August 22, 2001 1631 **U.S. PATENT DOCUMENTS EXAMINER** DOCUMENT INITIAL DATE NAME **CLASS** SUB-FILING DATE NUMBER CLASS AA3 AB3 AC3 AD3 AE3 AF3 AG3 AH3 AI3 **FOREIGN PATENT DOCUMENTS EXAMINER** INITIAL DOCUMENT NUMBER CLASS DATE COUNTRY SUB-**TRANSLATION CLASS** AJ3 Yes No AK3 Yes No AL3 Yes No AM3 Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Agrafiotis, D., "Theoretical Aspects of the Complex: Arts and New Technologies," Applications and Impacts AN 3 Information Processing '94, North-Holland, Vol. II, 1994, pp. 714-719. CAM Biswas, G. et al., "Evaluation of Projection Algorithms," IEEE Transactions On Pattern Analysis And Machine AO 3 Intelligence, IEEE Computer Society, Vol. PAMI-3, No. 6, November 1981, pp. 701-708. Bonchev, D. and Trinajstić, N., "Information theory, distance matrix, and molecular branching," *The Journal of Chemical Physics*, American Institute of Physics, Vol. 67, No. 10, November 15, 1977, pp. 4517, 4520-4533. AP 3 Chang, C.L. and Lee, R.C.T., "A Heuristic Relaxation Method for Nonlinear Mapping in Cluster Analysis," IEEE AQ 3 Transactions on Systems, Man, and Cybernetics, IEEE Systems, Man, and Cybernetics Society, Vol. SMC-3, March 1973, pp. 197-200. Cramer, R.D. et al., "Virtual Compound Libraries: A New Approach to Decision Making in Molecular Discovery AR 3 Research," J. Chem. Inf. Comput. Sci., American Chemical Society, Vol. 38, No. 6, November/December 1998. pp. 1010-1023. **EXAMINER** DATE CONSIDERED 18,2004

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FOURTH SUPPLEMENTAL INFORMATION
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SUPPLEMENTAL INFORMATION

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Page 26 of 37 APPLICATION NO. ATTY. DOCKET NO. 09/934,084 1503.1070003 FORM PTO-1449 APPLICANTS Lobanov et al. FOURTH SUPPLEMENTAL INFORMATION GROUP FILING DATE DISCLOSURE STATEMENT August 22, 2001 1631 **U.S. PATENT DOCUMENTS EXAMINER** CLASS SUB-FILING DATE DOCUMENT DATE NAME INITIAL CLASS NUMBER **AA26 AB26** AC26 AD26 AE26 AF26 AG26 AH26 AI26 **FOREIGN PATENT DOCUMENTS** EXAMINER COUNTRY **CLASS** SUB-TRANSLATION DOCUMENT NUMBER DATE INITIAL **CLASS** Yes AJ26 No Yes AK26 No Yes AL26 No Yes **AM26** No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Ghose, A. K. and Crippen, G.M., "Use of Physicochemical Parameters in Distance Geometry and Related Three-Dimensional Quantitative Structure-Activity Relationships: A Demonstration Using Escherichia coli ΑN <u> 26</u> Dihydrofolate Reductase Inhibitors", Journal of Medicinal Chemistry, American Chemical Society, Vol. 28, No. 3, CSM 1985, pp. 333-346. Good, A. C. et al., "Structure-Activity Relationships from Molecular Similarity Matrices", Journal of Medicinal AO 26 Chemistry, American Chemical Society, Vol. 36, No. 4, February 19, 1993, pp. 433-438. Gordon, E. M. et al., "Applications of Combinatorial Technologies to Drug Discovery. 2. Combinatorial Organic Synthesis, Library Screening Strategies, and Future Directions", Journal of Medicinal Chemistry, American ΑP 26 Chemical Society, Vol. 37, No. 10, May 13, 1994, pp. 1385-1401. Hartigan, J. A., "Representation of Similarity Matrices By Trees", Journal of the American Statistical Association, AQ <u>26</u> Vol. 62, No. 320, December, 1967, pp. 1140-1158. Hopfinger, A. J., "A QSAR Investigation of Dihydrofolate Reductase Inhibition by Baker Triazines Based upon AR Molecular Shape Analysis", Journal of the American Chemical Society, American Chemical Society, Vol. 102, <u>26</u> No. 24, November 19, 1980, pp. 7196-7206. DATE **EXAMINER** 1 200<u>4</u> **EXAMINER:** Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in

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Page 27 of 37 APPLICATION NO. ATTY. DOCKET NO. 09/934,084 1503.1070003 FORM PTO-1449 APPLICANTS Lobanov et al. FOURTH SUPPLEMENTAL INFORMATION GROUP FILING DATE DISCLOSURE STATEMENT 1631 August 22, 2001 U.S. PATENT DOCUMENTS **EXAMINER** FILING DATE CLASS SUB-NAME DATE DOCUMENT INITIAL CLASS NUMBER **AA27 AB27** AC27 AD27 AE27 AF27 AG27 **AH27 AI27** FOREIGN PATENT DOCUMENTS **EXAMINER** COUNTRY CLASS SUB-TRANSLATION DOCUMENT NUMBER DATE INITIAL CLASS Yes AJ27 No Yes **AK27** No Yes AL27 No Yes **AM27** No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Jackson, R. C., "Update on computer-aided drug design", Current Opinion in BIOTECHNOLOGY, Current ΑN <u>27</u> CADA Biology Ltd., Vol. 6, No. 6, December 1995, pp. 646-651. Kim, K. H., "Comparative molecular field analysis (CoMFA)", Molecular Similarity in Drug Design, ed. P. M. AO <u>27</u> Dean, Blackie Academic & Professional, 1995, Ch. 12, pp. 291-331. Kohonen, T., "Self-Organized Formation of Topologically Correct Feature Maps", Biological Cybernetics, AP 27 Springer-Verlag, Vol. 43, No. 1, 1982, pp. 59-69. Koile, K. and Shapiro, R., "Building A Collaborative Drug Design System", Proceedings of the 25h Hawaii ΑQ <u>27</u> International Conference on System Sciences, IEEE, 1992, pp. 706-716. Kowalski, B. R. and Bender, C. F., "Pattern Recognition. II. Linear and Nonlinear Methods for Displaying Chemical Data", Journal of the American Chemical Society, American Chemical Society, Vol. 95, No. 3, AR <u>27</u> February, 7, 1973, pp. 686-693. DATE ON NOTICE REPORTED **EXAMINER** 

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Page 28 of 37 ATTY. DOCKET NO. APPLICATION NO. 1503.1070003 09/934,084 FORM PTO-1449 APPLICANTS Lobanov et al. FOURTH SUPPLEMENTAL INFORMATION DISCLOSURE STATEMENT FILING DATE GROUP August 22, 2001 1631 **U.S. PATENT DOCUMENTS EXAMINER** SUB-FILING DATE **CLASS** DOCUMENT DATE NAME INITIAL NUMBER CLASS **AA28** AB28 AC28 AD28 AE28 AF28 AG28 AH28 AI28 **FOREIGN PATENT DOCUMENTS EXAMINER** INITIAL DOCUMENT NUMBER DATE COUNTRY CLASS SUB-TRANSLATION **CLASS** AJ28 Yes No **AK28** Yes No Yes AL28 No AM28 Yes No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Kruskal, J. B., "Nonmetric Multidimensional Scaling: A Numerical Method", Psychometrika, Vol. 29, No. 2, June, AN 28 1964, pp. 115-129. CSM Lengauer, T. and Rarey, M., "Computational methods for biomolecular docking", Current Opinion in Structural AO 28 Biology, Current Biology Ltd, Vol. 6, No. 3, June, 1996, pp. 402-406. Luke, B. T., "Evolutionary Programming Applied to the Development of Quantitative Structure-Activity AP <u>28</u> Relationships and Quantitative Structure-Property Relationships", Journal of Chemical Information and Computer Sciences, American Chemical Society, Vol. 34, No. 6, November/December 1994, pp. 1279-1287. Martin, E. J. et al., "Does Combinatorial Chemistry Obviate Computer-Aided Drug Design?", Reviews in AQ <u>28</u> Computational Chemistry, VCH Publishers, Inc., Vol. 10, 1997, pp. 75-99. Martin, E. J. et al., "Measuring Diversity: Experimental Design of Combinatorial Libraries for Drug Discovery", AR 28 Journal of Medicinal Chemistry, American Chemical Society, Vol. 38, No. 9, April 28, 1995, pp. 1431-1436.

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**EXAMINER** 

APPLICATION NO.

09/934,084

FORM PTO-1449

APPLICANTS Lobanov et

ATTY. DOCKET NO. 1503.1070003

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ATTY. DOCKET NO. 1503.1070003	APPLICATION NO. 09/934,084
APPLICANTS Lobanov et al.	
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Page 36 of 37 APPLICATION NO. ATTY. DOCKET NO. 09/934,084 1503.1070003 FORM PTO-1449 APPLICANTS Lobanov et al. OURTH SUPPLEMENTAL INFORMATION GROUP FILING DATE DISCLOSURE STATEMENT 1631 August 22, 2001 **U.S. PATENT DOCUMENTS EXAMINER** CLASS SUB-FILING DATE NAME DATE **DOCUMENT** INITIAL CLASS NUMBER **AA36 AB36** AC36 AD36 2003 R O YAM AE36 AF36 TECH CENTER 1600/2900 AG36 **AH36** AI36 FOREIGN PATENT DOCUMENTS **EXAMINER TRANSLATION** CLASS SUB-COUNTRY DOCUMENT NUMBER DATE INITIAL CLASS Yes AJ36 No Yes AK36 Νo Yes AL36 No Yes AM36 No OTHER (Including Author, Title, Date, Pertinent Pages, etc.) Crippen, G.M. and Havel, T.F., Distance Geometry and Molecular Conformation, Research Studies Press Ltd., AN 36 1988, entire book submitted. CSM Feuston, B. et al., "Comparison of Knowledge-Based and Distance Geometry Approaches for Generation of Molecular Conformations," Journal of Information and Computer Sciences, American Chemical Society, Vol. 41, AO <u>36</u> No. 3, 2001, pages 754-763. Ferguson, D. and Raber, D., "A New Approach to Probing Conformational Space with Molecular Mechanics: Random Incremental Pulse Search," Journal of the American Chemical Society, American Chemical Society, AΡ <u>36</u> Vol. 111, No. 12, 1989, pages 4371-4378. Halgren, T. and Nachbar, R., "Merck Molecular Force Field. IV. Conformational Energies and Geometries for MMFF94\*," Journal of Computational Chemistry, John Wiley & Sons, Inc., Vol. 17, Nos. 5 & 6, 1996, pages 587-AQ 36 915. Halgren, T., "Merck Molecular Force Field. V. Extension of MMFF94 Using Experimental Data, Additional Computational Data, and Empirical Rules\*," Journal of Computational Chemistry, John Wiley & Sons, Inc., Vol. AR <u>36</u> 17, Nos. 5 & 6, April 1996, pages 616-641. DATE CONSIDERED **EXAMINER** 2004 **EXAMINER**: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in

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# **ELECTRONIC INFORMATION DISCLOSURE STATEMENT**

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> Title of Invention

Method, System and Computer Program Product for **Determining Properties of Combinatorial Library Products** from Features of Library Building Blocks

MAY 0 5 2003

TECH CENTER 1600/2900

Application Number:

09/934084

Confirmation Number:

7373

First Named Applicant:

Victor Lobanov

Attorney Docket Number: 1503.1070003

Art Unit:

1631

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Note: Applicant is not required to submit a paper copy of cited US Patent Documents

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Electronic Version v18
Stylesheet Version v18.0

Title of Invention

Method, System and Computer Program Product for Determining Properties of Combinatorial Library Products from Features of Library Building Blocks

**Application Number:** 

09/934084

Confirmation Number:

7373

First Named Applicant:

Victor Lobanov

Attorney Docket Number: 1503.1070003

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Note: Applicant is not required to submit a paper copy of cited US Patent Documents

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### INFORMATION DISCLOSURE STATEMENT

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APPLICANTS Lobanov et al.	
FILING DATE August 22, 2001	GROUP 1631

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